Neural Network Data Interpretation

General Overview

The neural network software SLM is used to determine the concentrations of three Aroclors in the data generated from an environmental sample. Aroclors are mixtures of polychlorinated biphenyls. The input to the neural network system is a table of retention times and peak areas obtained from the raw signal that is generated by the gas chromatograph (GC) instrument. An artificial neural network (ANN) is used to establish the distinctive relationships between retention times, peak areas, and Aroclor concentration. When data from environmental samples are presented to the ANN, the output concentrations are based on interpolation from the training calibration standards.

Environmental Protection Agency (EPA) Method

SW-846 method 8080

Standard Analysis Method(SAM)

This SLM will support any SAM System using a GC.

Advantages

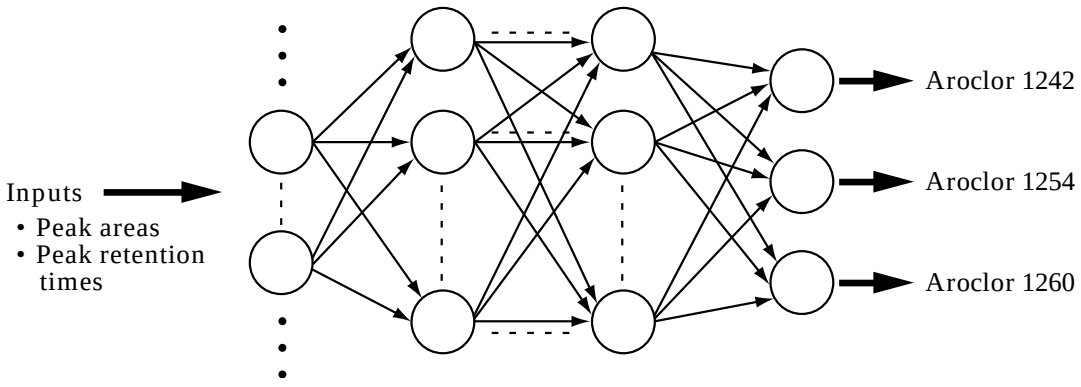
An analysis with the ANN potentially offers an advantage in the determination of samples containing mixtures of Aroclors. Manual data analysis of samples with mixtures of Aroclors is time-consuming and error prone. With the ANN many more possible combinations and patterns can be encoded into the network structure for a more automated and consistent analysis.

General Description of the Neural Network

The ANN concentration module analyzes the chromatograms produced by the GC and generates an assessment of the actual concentration and confidence intervals of the Aroclors contained in the environmental sample. Under normal operations, a table of retention times along with the corresponding peak areas is used as input into the software program. The ANN then computes the concentration parameters based on both linear and nonlinear combinations of the input values. The figure shows the basic structure of the ANN system, with multiple summation and transfer function nodes at multiple levels and weighted interconnects between nodes.

In the calibration and training node, the ANN is presented with a set of peak areas generated from a known concentration sample, and the output is compared to the true concentration. Based on the errors between the true and computed concentrations, the connection weights are adjusted to achieve the optimal reduction in concentration errors. Once the general relationships between the peak areas have been established, a calibration step converts the ANN output to actual concentrations. This step can be performed without retraining the entire network.

Figure 1. Basic structure of the ANN system.



Status

Under development.

Industrial Partner

SciBus Analytical, Inc.

Developers

This work is being conducted in the Electrical and Computer Engineering Department and the Robotics Research Laboratory of the University of Tennessee, Knoxville, Tennessee.

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